A Reduced Basis Method with Exact-Solution Certificates for Steady Symmetric Coercive Equations

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Abstract

We introduce a reduced basis method that computes rigorous upper and lower bounds of the energy associated with the infinite-dimensional weak solution of parametrized steady symmetric coercive partial differential equations with piecewise polynomial forcing and operators that admit decompositions that are affine in functions of parameters. The construction of the upper bound appeals to the standard primal variational argument; the construction of the lower bound appeals to the complementary variational principle. We identify algebraic conditions for the reduced basis approximation of the dual variable that results in an exact satisfaction of the dual feasibility conditions and hence a rigorous lower bound. The formulation permits an offline-online computational decomposition such that, in the online stage, the approximation and exact certificates can be evaluated in complexity independent of the underlying finite element discretization. We demonstrate the technique in two numerical examples: a one-dimensional reaction-diffusion problem with a parametrized diffusivity constant; a planar linear elasticity problem with a geometry deformation. We confirm in both cases that the method produces guaranteed upper and lower bounds of the energy at any parameter value, for any finite element discretization, and for any reduced basis approximation.

Keywords: reduced basis, *a posteriori* error bound, complementary variational principle, partial differential equations

1. Introduction

The theory and applications of the certified reduced basis method — a model reduction technique that aims to achieve a rapid and reliable characterization of parametrized partial differential equations — have advanced considerably in the past decade (see Rozza *et al.* [15], Quarteroni *et al.* [13], and references therein). A computationally efficient offline-online construction of error bounds has been one of the main focuses of the certified reduced basis method; however, to our knowledge, with few recent exceptions [18, 20], the existing reduced basis error bounds are with respect to some finite element "truth" which is *assumed* to be sufficiently accurate. This assumption may not be true for problems with spatial singularities and in any event is often not verified in a rigorous manner. The lack of reliable feedback on the validity of the "truth" can lead to either an inaccurate reduced basis prediction in the online stage (with respect to the infinite-dimensional

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14. ABSTRACT

We introduce a reduced basis method that computes rigorous upper and lower bounds of the energy associated with the in nite-dimensional weak solution of parametrized steady symmetric coercive partial di erential equations with piecewise polynomial forcing and operators that admit decompositions that are a ne in functions of parameters. The construction of the upper bound appeals to the standard primal variational argument; the construction of the lower bound appeals to the complementary variational principle. We identify algebraic conditions for the reduced basis approximation of the dual variable that results in an exact satisfaction of the dual feasibility conditions and hence a rigorous lower bound. The formulation permits an o ine-online computational decomposition such that, in the online stage, the approximation and exact certi cates can be evaluated in complexity independent of the underlying nite element discretization. We demonstrate the technique in two numerical examples: a one-dimensional reaction-di usion problem with a parametrized di usivity constant; a planar linear elasticity problem with a geometry deformation. We con rm in both cases that the method produces guaranteed upper and lower bounds of the energy at any parameter value, for any nite element discretization, and for any reduced basis approximation.

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weak solution) or overly conservative finite element "truth" and expensive computation in the offline stage. In this work, we introduce a reduced basis method that provides rigorous upper and lower bounds of the energy associated with the infinite-dimensional weak solution of parametrized steady symmetric coercive partial differential equations under two assumptions: the equation of interest consists of piecewise polynomial forcing functions (or "data"); the differential operator and data admit decompositions that are affine in functions of the parameters. We hence aim to entirely remove the issue of the "truth" within the certified reduced basis framework.

Our reduced basis method appeals to the complementary variational principle (or constitutive relation error), a principle that has been successfully used in the construction of finite element error bounds by, for instance, Ladevèze and Leguillion [7], Ainsworth and Oden [1], and Sauer-Budge *et al.* [16, 17]. More recently, in the context of model reduction, the principle has been used in the construction of rigorous error bounds for the proper generalized decomposition by Ladevèze and Chamoin [6]; the principle has also been applied to computational homogenization by Kerfrieden *et al.* [5]. In the context of certified reduced basis method for *parametrized* partial differential equations, the key to the application of the complementary variational principle is the identification of algebraic conditions for the dual reduced basis space associated with an *arbitrary parameter value*. In particular, the construction of the dual reduced basis space must be independent of the finite element complexity. We will demonstrate that this is indeed possible under the usual reduced basis assumption of the affine parameter dependence.

The contribution of the paper is the reduced basis formulation that provides upper and lower bounds for the energy associated with the infinite-dimensional weak solution of steady symmetric coercive equations. The bounds are uniform, as opposed to asymptotic, and certifies the approximation for any parameter value, for any finite element resolution, and for any reduced basis resolution. In addition, for our particular bound construction, we may associate the bound gap of the energy with the energy norm of the reduced basis solution error, and hence the energy bound provides an exact certificate of the solution field. The method admits an offline-online computational decomposition such that the online computational cost, including the cost associated with the bound computation, is independent of the underlying finite element discretization. As mentioned above, the formulation removes the issue of the finite element "truth" in the reduced basis certification process; the formulation is particularly suited for problems that exhibit spatial singularity in which the reliability of the finite element "truth" space can be questionable.

Before we proceed, we note limitations of the proposed bound strategy based on the complementary variational principle; the first three are inherited from the finite element counterpart. First, the method applies only to symmetric coercive problems. Second, the method requires the "data" — both from the interior forcing and boundary conditions — that is exactly representable as piecewise polynomials with respect to the underlying finite element triangulation. Third, the formulation requires, in the offline stage, a non-standard finite element approximation of the dual-feasible solution. Fourth, the formulation requires, in the online stage, a potentially large algebraic expansion, which could compromise the online efficiency. We discuss potential extensions that could remedy some of these limitations at the conclusion of this paper in Section 5.

This paper is organized as follows. In Section 2, we introduce our reduced basis method with exact-solution certificates for a diffusion equation with a parametrized diffusivity tensor; we recall the complementary variational principle, review a computational strategy for the dual variables, and present an offline-online computational strategy for the reduced basis method. In Section 3 we consider various extensions of the method: we consider a parametrized right-hand side, multiple

domain-dependent parameters, reaction-diffusion equation, (planar) linear elasticity equations, and affine geometry transformations. In Section 4, we demonstrate the method on two examples: one-dimensional reaction-diffusion equation with a variable diffusivity constant; planar-stress linear elasticity with an affine geometry transformation. In Section 5, we summarize the key contributions and identify several future research directions.

2. A Reduced Basis Method with Exact-Solution Certificates

2.1. Model Problem: Parametrized Diffusion Equation

By way of preliminaries, we first introduce a Lipschitz domain $\Omega \subset \mathbb{R}^d$ with a boundary partition $\partial\Omega = \Gamma_D \cup \Gamma_N$ for Γ_D non-empty. We then introduce a Hilbert space $V \equiv \{v \in H^1(\Omega) : v|_{\Gamma_D} = 0\}$ over Ω endowed with an inner product $(w, v)_V \equiv \int_\Omega \nabla w \cdot \nabla v dx$ and the induced norm $\|w\|_V = \sqrt{(w, w)_V}$. We next introduce a parameter space $\mathcal{D} \subset \mathbb{R}^P$. We then consider the following parametrized elliptic problem: given $\mu \in \mathcal{D}$, find $u(\mu) \in V$ such that

$$a(u(\mu), v; \mu) = \ell(v), \quad \forall v \in V,$$

where

$$a(w, v; \mu) \equiv \int_\Omega \nabla v \cdot D(\mu) \nabla w dx, \quad \forall w, v \in V,$$
$$\ell(v) \equiv \int_\Omega f v dx + \int_{\Gamma_N} g v ds, \quad \forall v \in V,$$

for $D(\mu) \in \mathbb{R}^{d\times d}$ a symmetric positive definite matrix (that is invariant over Ω), $f \in L^2(\Omega)$, and $g \in L^2(\Gamma_N)$. We assume that $D(\mu)$ permits a decomposition that is affine in functions of parameters: $D(\mu) = \sum_{q=1}^{Q} \Theta^q(\mu) D^q$ for parameter-dependent functions Θ^q: $\mathcal{D} \to \mathbb{R}$ and parameter-independent matrices $D^q \in \mathbb{R}^{d\times d}$, $q = 1, \ldots, Q$. We in addition assume that the data f and g admit piecewise polynomial representations of a degree at most p_f over Ω and Γ_N, respectively. Recall that the solution $u(\mu) \in V$ is the infimizer of an energy functional:

$$u(\mu) = \arg\inf_{w \in V} \mathcal{J}_p(w; \mu),$$

where

$$\mathcal{J}_p(w; \mu) \equiv \frac{1}{2} a(w, w; \mu) - \ell(w);$$

here the subscript "p" stands for "primal." We are interested in the energy associated with the exact solution $J(\mu) \equiv \mathcal{J}_p(u(\mu); \mu)$. We in particular consider an efficient construction of upper and lower bounds denoted by $J_N^+(\mu)$ and $J_N^-(\mu)$, respectively, *over the entire parametrer range*:

$$J_N^-(\mu) \le J(\mu) \le J_N^+(\mu), \quad \forall \mu \in \mathcal{D}.$$

We will later see that the above bounds, for our particular construction of $J_N^+(\mu)$, may be used to bound the energy norm of the error $|||u(\mu) - u_N(\mu)|||_\mu$ associated with a low-dimensional approximation $u_N(\mu)$ of the exact solution $u(\mu)$; here the energy norm is defined as $|||\cdot|||_\mu \equiv \sqrt{a(\cdot, \cdot; \mu)}$.

2.2. Certified Finite Element Method

2.2.1. Upper Bound

The construction of an upper bound of the exact energy $J(\mu)$ is straightforward owing to the variational structure of the elliptic problem. We first introduce a triangulation $\mathcal{T}_h$ of Ω and denote the skeleton of the triangulation by $\partial\mathcal{T}_h$; we require $\mathcal{T}_h$ to be chosen such that $f|_\kappa \in \mathbb{P}^{p_f}(\kappa)$, $\forall \kappa \in \mathcal{T}_h$, and $g|_\gamma \in \mathbb{P}^{p_f}(\gamma)$, $\forall \gamma \in \partial\mathcal{T}_h$. Here, $\mathbb{P}^p(D)$ denotes the space of polynomials of degree at most p over a domain D. We then introduce a $\mathcal{N}$-dimensional subspace $V^\mathcal{N} \equiv \{v \in V : v|_\kappa \in \mathbb{P}^p(\kappa),\ \forall \kappa \in \mathcal{T}_h\}$ on the triangulation $\mathcal{T}_h$. We seek the finite element approximation: given $\mu \in \mathcal{D}$, find

$$u^\mathcal{N}(\mu) \equiv \arg\inf_{w^\mathcal{N} \in V^\mathcal{N}} \mathcal{J}_p(w^\mathcal{N}; \mu) \ ;$$

recall that the infimizer is the solution of the weak statement: find $u^\mathcal{N}(\mu) \in V^\mathcal{N}$ such that

$$a(u^\mathcal{N}(\mu), v; \mu) = \ell(v) \ , \quad \forall v \in V^\mathcal{N} \ .$$

We now note that

$$J^{+,\mathcal{N}}(\mu) \equiv \mathcal{J}_p(u^\mathcal{N}(\mu); \mu) = \inf_{w^\mathcal{N} \in V^\mathcal{N}} \mathcal{J}_p(w^\mathcal{N}; \mu) \geq \inf_{w \in V} \mathcal{J}_p(w; \mu) = J(\mu) \ ;$$

thus, for any given $\mu \in \mathcal{D}$, $J^{+,\mathcal{N}}(\mu)$ is an upper bound of the exact energy $J(\mu)$. The superscript "$+,\mathcal{N}$" on $J^{+,\mathcal{N}}(\mu)$ signifies that the quantity is an *upper* bound computed in a $\mathcal{N}$-dimensional finite element space. We note that, owing to the piecewise polynomial assumption on f and g, the interior and boundary data can be integrated exactly and hence we do not commit variational crimes in the upper bound construction. The computational complexity of the upper bound construction is $\mathcal{O}(\mathcal{N}^k)$, where the exponent $k \geq 1$ dependents on the linear solver strategy.

2.2.2. Lower Bound: Principle

We now construct a lower bound of the exact energy $J(\mu)$. Towards this end, we first introduce a bilinear form

$$b(q, w) = \int_\Omega q \cdot \nabla w dx, \quad \forall q \in (L^2(\Omega))^d,\ \forall w \in V.$$

We then introduce a broken space defined on the triangulation $\mathcal{T}_h$,

$$\hat{V} \equiv \{v \in L^2(\Omega) : v|_\kappa \in H^1(\kappa),\ \forall \kappa \in \mathcal{T}_h\} \supset V. \tag{1}$$

We next define a space of vector-valued functions $\hat{Y} \equiv (\hat{V})^d$. We then introduce a space of dual variables that plays a key role in the certification procedure,

$$Q \equiv \{q \in \hat{Y} : b(q, w) = \ell(w),\ \forall w \in V\};$$

for a reason that becomes clear shortly, we refer to the condition $b(q, w) = \ell(w)$, $\forall w \in V$, as the dual feasibility condition. We finally introduce a dual energy functional

$$\mathcal{J}_d(q; \mu) \equiv -\frac{1}{2} \int_\Omega q \cdot D^{-1}(\mu) q dx, \quad \forall q \in \hat{Y};$$

here the subscript "d" stands for "dual."

We now state the key proposition for our lower bound construction:

Proposition 1. For any $q \in Q$ and $\mu \in \mathcal{D}$,

$$J(\mu) \geq \mathcal{J}_d(q;\mu) \ .$$

Proof. By the complementary variational principle,

$$\begin{aligned}
0 &\leq \frac{1}{2}\sum_{\kappa\in\mathcal{T}_h}\int_\kappa (q - D(\mu)\nabla w)\cdot D^{-1}(\mu)(q - D(\mu)\nabla w)dx \\
&= \frac{1}{2}\int_\Omega q\cdot D^{-1}(\mu)qdx + \frac{1}{2}\sum_{\kappa\in\mathcal{T}_h}\int_\kappa \nabla w\cdot D(\mu)\nabla w dx - \sum_{\kappa\in\mathcal{T}_h}\int_\kappa q\cdot\nabla w dx \\
&= -\mathcal{J}_d(q;\mu) + \frac{1}{2}a(w,w) - b(q,w) \\
&= -\mathcal{J}_d(q;\mu) + \frac{1}{2}a(w,w) - \ell(w), \quad \forall q\in Q,\ \forall w\in V;
\end{aligned}$$

here the last equality follows from the definition of the dual space Q. Since $u(\mu) \in V$, it follows that

$$\mathcal{J}_d(q;\mu) \leq \frac{1}{2}a(u(\mu),u(\mu)) - \ell(u(\mu)) = J(\mu), \quad \forall q\in Q \ ,$$

which is the desired relationship. □

The proposition suggests that, if we can efficiently construct the dual space Q, then we may use any element of Q to construct a lower bound. In addition, as regard its sharpness, we may appeal to

Proposition 2. The lower bound estimate is sharp in the sense that

$$\sup_{q\in Q}\mathcal{J}_d(q;\mu) = J(\mu).$$

Proof. We set $p(\mu) = D(\mu)\nabla u(\mu)$. We readily confirm that $p(\mu) \in Q$ because

$$b(p(\mu),w) = b(D(\mu)\nabla u(\mu),w) = a(u(\mu),w) = \ell(w), \quad \forall w\in V.$$

In addition,

$$\mathcal{J}_d(p(\mu);\mu) = -\frac{1}{2}\int_\Omega \nabla u(\mu)\cdot D(\mu)\nabla u(\mu)dx = \frac{1}{2}\int_\Omega \nabla u(\mu)\cdot D(\mu)\nabla u(\mu)dx - \ell(u(\mu)) = J(\mu),$$

and hence $p(\mu) \in Q$ is the supremizer and the desired equality holds. □

In the construction of the reduced basis lower bound to be introduced in Section 2.3, we will only appeal to the fact that an element in Q that approximates $p(\mu)$ is computable in the offline stage. In other words, our reduced basis lower bound does not rely on a particular finite element approximation procedure for $p(\mu)$. However, in below for completeness, we review a finite-element approximation strategy for $p(\mu)$ that exactly satisfies the dual feasibility condition. (See also Pled *et al.* [12] for other approximation strategies.)

2.2.3. Lower Bound: Localization by Relaxation

We wish to construct an approximation of the exact flux $p(\mu) \in Q$ in a computationally efficient manner; here we follow the approach of Sauer-Budge *et al.* [16] which employs a two-stage procedure: the computation of an approximate inter-elemental flux; the maximization of localized dual problems with the exact dual feasibility constraint.

Towards this end, we consider an elemental decomposition of the dual feasibility constraint for the space Q:

$$\begin{aligned}\ell(w) - b(q,w) &= \int_\Omega f w dx + \int_{\Gamma_N} g w ds - \sum_{\kappa\in\mathcal{T}_h} \int_\kappa q \cdot \nabla w dx \\ &= \sum_{\kappa\in\mathcal{T}_h} \left[\int_\kappa (f + \nabla\cdot q) w dx - \int_{\partial\kappa\setminus\Gamma_N} (n_\kappa \cdot q) w ds + \int_{\partial\kappa\cap\Gamma_N} (g - n_\kappa\cdot q) w ds \right], \quad \forall w \in V \ .\end{aligned}$$

Note that sufficient conditions to satisfy the constraints are, in the sense of distribution,

$$-\nabla\cdot q = f \quad \text{in } H^{-1}(\kappa),\ \forall\kappa\in\mathcal{T}_h, \tag{2}$$

$$\hat{n}_\kappa \cdot q = g \quad \text{in } H^{-1/2}(\partial\kappa\cap\Gamma_N),\ \forall\kappa\in\mathcal{T}_h, \tag{3}$$

$$\hat{n}_\kappa\cdot q|_\kappa = \hat{n}_{\kappa'}\cdot q|_{\kappa'} \quad \text{in } H^{-1/2}(\bar{\kappa}\cap\bar{\kappa}'),\ \forall\kappa,\kappa'\in\mathcal{T}_h; \tag{4}$$

here $\bar{\kappa}$ denotes the closure of κ, and hence $\bar{\kappa}\cap\bar{\kappa}'$ is the face shared by the elements κ and κ'. The last condition requires the continuity of the normal fluxes across elemental interfaces, which introduces a global coupling. In order to localize the problem, we now introduce a trace space on the skeleton of the triangulation $\partial\mathcal{T}_h$:

$$\Lambda \equiv \{\chi : \chi|_\gamma \in H^{-1/2}(\gamma)\ , \forall\gamma\in\partial\mathcal{T}_h;\ \chi|_\gamma = g,\ \forall\gamma\in\Gamma_N\}\ .$$

We then note that, if we introduce an arbitrary fixed element $\chi\in\Lambda$, we may enforce the flux condition on Neumann boundaries (3) and the normal flux continuity constraint (4) by

$$\hat{n}_\kappa\cdot q|_\kappa = \sigma_\kappa\chi \quad \text{in } H^{-1/2}(\partial\kappa),\ \forall\kappa\in\mathcal{T}_h\ . \tag{5}$$

Here σ_κ is a function over each elemental face of $\kappa\in\mathcal{T}_h$ and, for a face shared with $\kappa'\in\mathcal{T}_h$ and for an arbitrary ordering of the elements,

$$\sigma_\kappa = \begin{cases} -1, & \kappa < \kappa', \\ 1, & \text{otherwise} \end{cases} \quad ;$$

for a face on Γ_N, $\sigma_\kappa = 1$. In words, χ specifies the inter-elemental flux for every face of the triangulation, which in turn ensures the continuity of the inter-elemental normal flux.

We may express this form of the space $\hat{Q}(\chi)\subset Q$, characterized by the interface flux χ, in a more convenient form. We first introduce a broken bilinear form

$$\hat{b}(q,w) = \sum_{\kappa\in\mathcal{T}_h}\int_\kappa q\cdot\nabla\hat{w}dx, \quad \forall q\in(L^2(\Omega))^d,\ \forall\hat{w}\in\hat{V},$$

where we recall $\hat{V}$ is the broken space defined in (1). We next introduce a "jump" bilinear form

$$\hat{c}(\hat{w},\chi) = \sum_{\kappa\in\mathcal{T}_h} \int_{\partial\kappa} \sigma_\kappa \hat{w}\chi ds, \quad \forall \hat{w}\in\hat{V},\ \forall\chi\in\Lambda\ .$$

We finally define

$$\hat{Q}(\chi) \equiv \{q\in\hat{Y} : \hat{b}(q,\hat{w}) = \ell(\hat{w}) + \hat{c}(\hat{w},\chi),\ \forall\hat{w}\in\hat{V}\}\ .$$

Note that, in order to ensure that the space is not empty, the interface flux $\chi\in\Lambda$ must be equilibrating in the sense that $0 = \ell(\mathbf{1}_\kappa) + c(\mathbf{1}_\kappa,\chi)$, $\forall\kappa\in\mathcal{T}_h$, where $\mathbf{1}_\kappa = 1$ on κ and $\mathbf{1}_\kappa = 0$ on $\Omega\setminus\kappa$. We emphasize that $\hat{Q}(\chi)\subset Q$ for any equilibrating flux $\chi\in\Lambda$.

2.2.4. Lower Bound: Computation

We now consider a finite element approximation of the interface flux $\lambda(\mu)\in\Lambda$ and the dual variable $p(\mu)\in\hat{Q}(\lambda(\mu))$. Towards this end, we first introduce a finite element flux space $\Lambda^{\mathcal{N}} \equiv \{\lambda\in\Lambda : \lambda|_\gamma\in\mathbb{P}^p(\gamma),\ \forall\gamma\in\partial\mathcal{T}_h\}$. (Note that the dimension of this space is not $\mathcal{N}$ but is of $\mathcal{O}(\mathcal{N})$.) We then seek an approximate interface flux associated with the finite element solution $u^{\mathcal{N}}(\mu)\in V^{\mathcal{N}}$: find $\lambda^{\mathcal{N}}(\mu)\in\Lambda$ such that

$$\hat{c}(\hat{w},\lambda^{\mathcal{N}}(\mu)) = a(u^{\mathcal{N}}(\mu),\hat{w};\mu) - \ell(\hat{w})\ , \quad \forall\hat{w}\in\hat{V}^{\mathcal{N}}\ . \tag{6}$$

We solve this so called equilibration problem using the method of Ladevèze and Leguillon [7] and in particular its high-order extension by Ainsworth and Oden [1], which has a computational cost that scales linearly with the number of finite element unknowns.

We next introduce a broken finite element space of interior fluxes: $\hat{Y}^{\mathcal{N}} \equiv (\hat{V}^{\mathcal{N}})^d$. We now wish to construct a dual-feasible subspace $\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu))\subset\hat{Q}(\lambda^{\mathcal{N}}(\mu))\subset Q$,

$$\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu)) \equiv \{q\in\hat{Y}^{\mathcal{N}} : b(q,\hat{w}) = \ell(\hat{w}) + c(\hat{w},\lambda^{\mathcal{N}}(\mu)),\ \forall\hat{w}\in\hat{V}\}\ . \tag{7}$$

We must satisfy *exactly* the dual feasibility condition (2), (3), and (4). We also recall that we may replace the constraints (3) and (4) by a single condition (5). Hence, the sufficient condition for dual feasibility in strong form is

$$\begin{aligned} -\nabla\cdot q &= f \quad \text{in } H^{-1}(\kappa), \quad \forall\kappa\in\mathcal{T}_h\ , \\ \hat{n}_\kappa\cdot q &= \sigma_\kappa\lambda^{\mathcal{N}}(\mu) \quad \text{in } H^{-1/2}(\partial\kappa), \quad \forall\kappa\in\mathcal{T}_h\ . \end{aligned}$$

Note that our volume data $f|_\kappa\in\mathbb{P}^{p_f}(\kappa)$ and boundary data $\lambda^{\mathcal{N}}(\mu)|_\gamma\in\mathbb{P}^p(\gamma)$, $\gamma\in\partial\kappa$. In addition, by our choice of the space for q, $\nabla\cdot q|_\kappa\in\mathbb{P}^{p-1}(\kappa)$. It follows that we need only test the equation over κ against the *finite*-dimensional space $\mathbb{P}^{p-1}(\kappa)$ (for $p\geq p_f+1$) and not the *infinite*-dimensional space $H^1(\kappa)$. Similarly, we need only test the equations over $\partial\kappa$ against *finite*-dimensional spaces $\mathbb{P}^p(\gamma)$, $\gamma\in\partial\kappa$. Thus, we can construct — implicitly using a *finite* number of constraints — the space $\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu))\subset Q$ that satisfies *exactly* the dual feasibility condition. The existence of at least one $q\in\hat{Y}^{\mathcal{N}}$ that satisfies the dual feasibility conditions, and hence the non-emptiness of $\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu))$, is discussed in [16].

We may now readily construct a finite element approximation of a lower bound of the energy. We first solve (6) for the approximate flux function $\lambda^{\mathcal{N}}(\mu)$ associated with the finite element solution $u^{\mathcal{N}}(\mu)$. We then compute the finite element approximation of the dual variable

$$p^{\mathcal{N}}(\mu) \equiv \underset{q^{\mathcal{N}}\in\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu))}{\arg\sup} \mathcal{J}_d(q^{\mathcal{N}};\mu)\ .$$

We finally evaluate the associated lower bound

$$J^{-,\mathcal{N}}(\mu) \equiv \mathcal{J}_d(p^{\mathcal{N}}(\mu);\mu) \leq J(\mu);$$

the inequality is a direct consequence of Proposition 1 and $\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu)) \subset Q$. The superscript "$-,\mathcal{N}$" on $J^{-,\mathcal{N}}(\mu)$ signifies that the quantity is a *lower* bound computed in a $\mathcal{O}(\mathcal{N})$-dimensional finite element space. Note that the dual maximization problem is a quadratic program with linear constraints, which reduces to element-wise saddle problems that can be solved efficiently. The computational complexities of the inter-elemental flux calculation and local dual problems are of $\mathcal{O}(\mathcal{N})$ (provided that the primal solution $u^{\mathcal{N}}(\mu)$, which is used in the calculation of $\lambda^{\mathcal{N}}(\mu)$, has already been computed).

2.3. Reduced Basis Method

2.3.1. Upper Bound

We now introduce a reduced basis method that provides rigorous upper and lower bounds of the exact energy. As before, the construction of an upper bound is straightforward owing to the variational structure of the elliptic equation. We first introduce a hierarchical N-dimensional reduced basis space

$$V_N \equiv \text{span}\{u^{\mathcal{N}}(\mu_{(n)}),\ \mu_{(n)} \in M_N\} \equiv \text{span}\{\xi_n^{\mathcal{N}}\}_{n=1}^N \subset V^{\mathcal{N}},$$

where $M_N \equiv \{\mu_{(n)}\}_{n=1}^N$ is the set of N reduced basis parameter points (for formally $N \leq \mathcal{N}$ but typically $N \ll \mathcal{N}$), and $\{\xi_n^{\mathcal{N}}\}_{n=1}^N$ is the orthonormal basis with respect to, say, $(\cdot,\cdot)_V$. Our reduced-basis approximation is given by

$$u_N(\mu) \equiv \arg\inf_{w_N \in V_N} \mathcal{J}_p(w_N;\mu)\ ;$$

again, the infimizer is given by the Galerkin statement: find $u_N(\mu) \in V_N$ such that

$$a(u_N(\mu), v_N;\mu) = \ell(v_N)\ , \quad \forall v_N \in V_N\ .$$

Our reduced basis upper bound is then given by

$$J_N^+(\mu) \equiv \mathcal{J}_p(u_N(\mu);\mu) = \inf_{w_N \in V_N} \mathcal{J}_p(w_N;\mu) \geq \inf_{w^{\mathcal{N}} \in V^{\mathcal{N}}} \mathcal{J}_p(w^{\mathcal{N}};\mu) = J^{+,\mathcal{N}}(\mu) \geq J(\mu)\ ;$$

The superscript and subscript "$\cdot_N^+$" on $J_N^+(\mu)$ signifies that the quantity is an *upper* bound computed in a N-dimensional reduced basis space. The reduced basis upper bound is looser than the finite element upper bound.

The computation of the reduced basis upper bounds permits the standard offline-online computational decomposition. (See, for example, Rozza *et al.* [15].) In the offline stage, we first solve N finite element problems to obtain basis functions $u^{\mathcal{N}}(\mu_{(n)})$, $n = 1,\ldots,N$, for the reduced basis space. We then orthonormalize the functions to obtain $\xi_n^{\mathcal{N}}$, $n = 1,\ldots,N$. We next appeal to the decomposition of the diffusion coefficient that is affine in functions of parameter and compute parameter-independent matrices $\hat{\mathbf{A}}_{ij} \in \mathbb{R}^{N\times N}$, $i,j = 1,\ldots,d$, and vector $\mathbf{F} \in \mathbb{R}^N$ with entries

$$(\hat{\mathbf{A}}_{ij})_{mn} = \int_\Omega \frac{\partial \xi_m}{\partial x_i}\frac{\partial \xi_n}{\partial x_j}dx, \quad m,n = 1,\ldots,N\ ,$$
$$\mathbf{F}_m = \ell(\xi_m), \quad m = 1,\ldots,N\ .$$

In the online stage, we take a three-step procedure. We first compute a parameter-dependent matrix

$$\mathbf{A}(\mu) \equiv \sum_{i,j=1}^{d} D_{ij}(\mu)\hat{\mathbf{A}}_{ij}.$$

We then solve a $N \times N$ reduced basis problem: find $\alpha_N^\star(\mu) \in \mathbb{R}^N$ such that

$$\mathbf{A}(\mu)\alpha_N^\star(\mu) = \mathbf{F}$$

We finally evaluate the reduced basis upper bound

$$J_N^+(\mu) = -\frac{1}{2}(\alpha_N^\star(\mu))^T \mathbf{A}(\mu)\alpha_N^\star(\mu) \ .$$

The computational complexity of the online stage is $\mathcal{O}(d^2N^2) + \mathcal{O}(N^3)$ and is in particular independent of the finite element complexity of $\mathcal{O}(\mathcal{N})$ (or the exact infinite-dimensional problem complexity of infinity).[1]

2.3.2. Lower Bound

We now construct a reduced basis approximation of the energy lower bound. We first define the reduced basis space associated with the dual variable

$$\hat{Y}_N \equiv \text{span}\{p^{\mathcal{N}}(\mu_{(n)}),\ \mu_{(n)} \in M_N\} \equiv \text{span}\{\eta_n^{\mathcal{N}}\}_{n=1}^N \subset \hat{Y}^{\mathcal{N}}.$$

Here, $\{\eta_n^{\mathcal{N}}\}_{n=1}^N$ is the orthonormal basis with respect to, say, $(\cdot,\cdot)_{(L^2(\Omega))^d}$; we in addition introduce the change of basis matrix $\omega \in \mathbb{R}^{N\times N}$ that satisfies

$$\eta_n^{\mathcal{N}} = \sum_{n'=1}^{N} p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}, \quad n = 1,\ldots,N.$$

We then define the key space for the lower bound computation: the reduced basis dual space with the dual feasibility constraint,

$$Q_N \equiv \{q \in \hat{Y}_N : b(q,w) = \ell(w),\ \forall w \in V\}\ ; \tag{8}$$

we again must satisfy *exactly* the dual feasibility conditions. Towards this end, we substitute the reduced basis approximation of the dual variable $p_N = \sum_{n=1}^N \eta_n^{\mathcal{N}}\beta_{Nn} = \sum_{n=1}^N\sum_{n'=1}^N p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}$ to express the dual feasibility condition (8) in terms of the reduced basis coefficients $\beta_N \in \mathbb{R}^N$:

$$b(p_N,w) = b(\sum_{n=1}^{N}\sum_{n'=1}^{N} p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}, w) = \ell(w), \quad \forall w \in V. \tag{9}$$

[1]The $\mathcal{O}(d^2N^2)$ term associated with the assembly process is an upper bound of the $\mathcal{O}(Q_aN^2)$ term associated with the "standard" expression for the reduced-basis assembly, where Q_a is the number of terms in the affine expansion of $a(\cdot,\cdot;\cdot)$ [15], for the spatially invariant diffusivity tensor $D(\mu) \in \mathbb{R}^{d\times d}$.

On the other hand, we appeal to the bilinearity of the form $b(\cdot,\cdot)$ and the fact that each $p^{\mathcal{N}}(\mu_{(n')}) \in Q$ — which implies $b(p^{\mathcal{N}}(\mu_{(n')}), w) = \ell(w)$, $\forall w \in V$, $n' = 1, \ldots, N$ — to obtain

$$b(\sum_{n=1}^{N}\sum_{n'=1}^{N} p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}, w) = \sum_{n=1}^{N}\sum_{n'=1}^{N} \omega_{n'n}\beta_{Nn} b(p^{\mathcal{N}}(\mu_{(n')}), w)$$
$$= \sum_{n=1}^{N}\sum_{n'=1}^{N} \omega_{n'n}\beta_{Nn}\ell(w), \quad \forall w \in V. \tag{10}$$

The comparison of (9) and (10) shows that the sufficient condition for $p_N \in Q_N$ is

$$\sum_{n=1}^{N}\sum_{n'=1}^{N} \omega_{n'n}\beta_{Nn} = 1.$$

With the constraint, the effective dimension of the reduced basis coefficient space is $N-1$. We now define our reduced basis energy lower bound as

$$J_N^-(\mu) \equiv \sup_{q_N \in Q_N} \mathcal{J}_d(q_N;\mu) = \sup_{\substack{q_N \in \hat{Y}_N \\ \sum_{n=1}^{N}\sum_{n'=1}^{N}\omega_{n'n}\beta_{Nn}=1}} \mathcal{J}_d(q_N;\mu);$$

The superscript and subscript "$\cdot_N^-$" on $J_N^-(\mu)$ signifies that the quantity is a *lower* bound computed in a N-dimensional reduced basis space. We note that the reduced basis lower bound, unlike the upper bound, can be tighter than the finite element lower bound. This is because the function $p_N(\mu)$ is optimized for the tightest bound from a set of dual feasible functions in $Q_N \subset Q$ whereas the finite element dual variable $p^{\mathcal{N}}(\mu)$ — computed by the procedure described in Section 2.2.4 — is chosen from a subspace $\hat{Q}^{\mathcal{N}}(\hat{\lambda}^{\mathcal{N}}(\mu)) \subset Q$ restricted by the choice of $\hat{\lambda}^{\mathcal{N}}(\mu)$.

The evaluation of the reduced basis lower bound also permits an offline-online computational decomposition. In the offline stage, we first solve N finite element dual problems to obtain basis functions $p^{\mathcal{N}}(\mu_{(n')})$, $n' = 1, \ldots, N$, for the reduced basis space $\hat{Y}_N$. We then orthonormalize the functions to obtain $\eta_n^{\mathcal{N}}$, $n = 1, \ldots, N$, and the change of basis matrix $\omega \in \mathbb{R}^{N\times N}$. We next sum the leading index of the change of basis matrix to form $\omega_n^{\text{sum}} \in \mathbb{R}^N$ with entries

$$\omega_n^{\text{sum}} \equiv \sum_{n'=1}^{N} \omega_{n'n}, \quad n = 1, \ldots, N.$$

We then compute parameter-independent matrices $\hat{\mathbf{K}}_{ij} \in \mathbb{R}^{N\times N}$, $i, j = 1, \ldots, d$, with entries

$$(\hat{\mathbf{K}}_{ij})_{mn} = \int_\Omega \eta_{m,i}^{\mathcal{N}} \eta_{n,j}^{\mathcal{N}} dx \ ,$$

where $\eta_{m,i}^{\mathcal{N}}$ denotes the i-th vector component of the m-th basis function.

In the online stage, we take a three-step procedure. We first form a parameter-dependent matrix $\mathbf{K}(\mu) \in \mathbb{R}^{N\times N}$ defined by

$$\mathbf{K}(\mu) \equiv \sum_{i,j=1}^{d} D_{ij}^{-1}(\mu)\hat{\mathbf{K}}_{ij}.$$

We then solve a $N \times N$ quadratic program with a single linear constraint

$$\beta_N^\star(\mu) = \underset{\substack{\beta_N \in \mathbb{R}^N \\ (\omega^{\text{sum}})^T \beta_N = 1}}{\arg\sup} \; -\frac{1}{2} \beta_N^T \mathbf{K}(\mu) \beta_N \; ,$$

which requires the solution of a $(N+1) \times (N+1)$ saddle system. We finally evaluate the lower bound

$$J_N^- = -\frac{1}{2} (\beta_N^\star(\mu))^T \mathbf{K}(\mu) \beta_N^\star(\mu) \; .$$

The computational complexity of the online stage is $\mathcal{O}(d^2 N^2) + \mathcal{O}((N+1)^3)$ and is in particular independent of the finite element complexity of $\mathcal{O}(\mathcal{N})$ (or the exact infinite-dimensional complexity of infinity).

Remark 1. Here we choose the same set of parameter values for the primal snapshots that spans V_N and the dual snapshots that spans $\hat{Y}_N$. In general the parameter values associated with the primal and dual snapshots need not be the same. In particular, for *online* efficiency — that is to reduce N — it is in general advantageous to consider different parameter values because the parametric manifold associated with the primal and dual solutions can be quite different. However, for *offline* efficiency, it is advantageous to consider the same snapshot parameter values because the computation of the finite element dual solution by the equilibration procedure requires the primal solution. We recall that the complexity of the primal solve is $\mathcal{O}(\mathcal{N}^k)$, $k \geq 1$, where as the complexity of the equilibration procedure is $\mathcal{O}(\mathcal{N})$.

2.3.3. Energy Norm of the Error

The upper and lower bounds of the energy functional may be used for the global certification of the reduced-basis solution in the energy norm $|||w|||_\mu \equiv \sqrt{a(w,w;\mu)}$:

Proposition 3. The upper and lower bound of the energy functional is related to the energy norm of the error in the sense that, for any $\mu \in \mathcal{D}$,

$$|||u(\mu) - u_N(\mu)|||_\mu^2 \leq 2(J_N^+(\mu) - J_N^-(\mu)) \; .$$

Proof. We appeal to the definition of the energy norm, Galerkin orthogonality, and the definition of the energy functional to obtain

$$\begin{aligned} |||u(\mu) - u_N(\mu)|||_\mu^2 &\equiv a(u(\mu) - u_N(\mu), u(\mu) - u_N(\mu); \mu) = a(u(\mu), u(\mu); \mu) - a(u_N(\mu), u_N(\mu); \mu) \\ &= -2\mathcal{J}_p(u(\mu); \mu) + 2\mathcal{J}_p(u_N(\mu); \mu) \leq 2(J_N^+(\mu) - J_N^-(\mu)) \; ; \end{aligned}$$

this concludes the proof. □

3. Extensions

3.1. Extension 1: Parametrized Right-Hand Side

We now consider an extension of the method for the case in which the right-hand side data $\ell(\cdot)$ is parametrized but permits a decomposition that is affine in functions of the parameter:

$$\ell(v;\mu) \equiv \sum_{s=1}^{S} \Theta_s(\mu) \ell_s(v) \tag{11}$$

for parameter-dependent functions $\Theta_s : \mathcal{D} \to \mathbb{R}$ and parameter-independent functionals $\ell_s \in V'$, $s = 1, \ldots, S$. The primal formulation requires no modifications, and the construction of the upper bound follows from the same variational argument as before.

To construct a lower bound, we appeal to the linearity of the dual solution $p(\mu)$ on the right hand side. We first note that the dual feasibility space is now parameter-dependent and is given by

$$Q_N(\mu) \equiv \{q \in \hat{Y}_N : b(q, w) = \sum_{s=1}^{S} \Theta_s(\mu)\ell_s(w),\ \forall w \in V\}. \tag{12}$$

We next substitute the form of our reduced basis approximation $p_N \equiv \sum_{n=1}^{N} \eta_n^{\mathcal{N}} \beta_{Nn} = \sum_{n=1}^{N}\sum_{n'=1}^{N} p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}$ to the expression for the constraint, appeal to the bilinearity of $b(\cdot,\cdot)$, and invoke $p^{\mathcal{N}}(\mu_{(n')}) \in Q(\mu_{(n')})$, $n = 1, \ldots, N$ — which implies $b(p^{\mathcal{N}}(\mu_{(n')}), w) = \sum_{s=1}^{S} \Theta_s(\mu)\ell_s(w)$, $\forall w \in V$, $n' = 1, \ldots, N$ — to obtain

$$b(\sum_{n=1}^{N}\sum_{n'=1}^{N} p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}, w) = \sum_{n=1}^{N}\sum_{n'=1}^{N} \omega_{n'n}\beta_{Nn} b(p^{\mathcal{N}}(\mu_{(n')}), w) \tag{13}$$

$$= \sum_{s=1}^{S}\sum_{n=1}^{N}\sum_{n'=1}^{N} \Theta_s(\mu_{(n')})\omega_{n'n}\beta_{Nn}\ell_s(w), \quad \forall w \in V. \tag{14}$$

The comparison of (12) and (14) shows that a sufficient condition for $p_N \in Q_N(\mu)$ is

$$\sum_{n=1}^{N}\sum_{n'=1}^{N} \Theta_s(\mu_{(n')})\omega_{n'n}\beta_{Nn} = \Theta_s(\mu), \quad s = 1, \ldots, S\ ;$$

the set of S constraints is a generalization of the single constraint $\sum_{n=1}^{N}\sum_{n'=1}^{N} \omega_{n'n}\beta_{Nn} = 1$ for the non-parametrized right-hand side case. Note that the effective dimension of the reduced basis space is $N - S$ (assuming the S constraints are linearly independent); we consequently require that $N \geq S$.

The offline-online computational decomposition follows from the non-parametrized right-hand side case with one exception: in the online stage, we simply impose S constraints instead of the single constraint. The computational complexity of the online stage is $\mathcal{O}(d^2N^2) + \mathcal{O}((N + S)^3)$, where $N + S$ is the size of the saddle system with the S constraints. Note that, as the effective dimension of the reduced basis space is $N - S$, the dimension N may need to be larger than the non-parametrized right-hand side case.

Remark 2. Instead of the procedure described above, we may construct S parameter-independent dual feasibility spaces, each corresponding to the specific ℓ_s. Specifically, we may construct separate spaces $Q_{s,N} \equiv \{q \in \hat{Y}_{s,N} : b(q, w) = \ell_s(w),\ \forall w \in V\}$, $s = 1, \ldots, S$, with $Y_{s,N} \equiv \text{span}\{p_s^{\mathcal{N}}(\mu_{(n)})\}_{n=1}^{N}$ associated with ℓ_s.

3.2. Extension 2: Multiple Domains

We now consider an extension of the method for the case in which the bilinear form $a(\cdot,\cdot)$ constitutes of contributions from K_{dom} subdomains, $\Omega^{(k)}$, $k = 1, \ldots, K_{\text{dom}}$:

$$a(w, v; \mu) \equiv \sum_{k=1}^{K_{\text{dom}}} \int_{\Omega^{(k)}} \nabla v \cdot D^{(k)}(\mu)\nabla w dx, \quad \forall w, v \in V;$$

we assume symmetric positive definite matrices $D^{(k)}(\mu) \in \mathbb{R}^{d\times d}$, $k = 1, \ldots, K_{\rm dom}$, are constant over each subdomain (but in general different across subdomains). The construction of the upper bound follows from the same variational argument, and the primal formulation requires no modifications.

To construct a lower bound, the dual energy functional is modified to

$$\mathcal{J}_d(q;\mu) \equiv -\frac{1}{2}\sum_{k=1}^{K_{\rm dom}} \int_{\Omega^{(k)}} q\cdot(D^{(k)}(\mu))^{-1} q dx \ .$$

With the redefinition, we may follow the proof of Proposition 1 and still show that

$$\mathcal{J}_d(q;\mu) \le J(\mu), \quad \forall q \in Q,$$

where $Q \equiv \{q \in \hat{Y} : b(q,w) = \ell(w),\ \forall w \in V\}$ as before. We in particular note that Q is independent of the diffusion coefficients $D^{(k)}(\mu)$, $k = 1, \ldots, K_{\rm dom}$. It follows that, for any given $\mu \in \mathcal{D}$, we may find a dual feasible function $p^{\mathcal{N}}(\mu) \in Q$ using the finite element procedure described in Section 2.2.4. In addition, the constraints for the reduced basis coefficients are unchanged: $\sum_{n=1}^{N}\sum_{n'=1}^{N} \omega_{n'n}\beta_{Nn} = 1$.

We need to make only minor modifications to the offline-online computational procedure. In the offline stage, we first solve N finite element dual problems to obtain snapshots $p^{\mathcal{N}}(\mu_{(n)})$, $n = 1, \ldots, N$. We then orthonormalize the functions to obtain the basis $\{\eta_n^{\mathcal{N}}\}_{n=1}^N$ for the reduced basis space $\hat{Y}_N$, and the change of basis matrix $\omega \in \mathbb{R}^{N\times N}$. We next compute parameter-independent matrices $\hat{\mathbf{K}}_{ij}^{(k)} \in \mathbb{R}^{N\times N}$, $i, j = 1, \ldots, d$, $k = 1, \ldots, K_{\rm dom}$, with entries

$$(\hat{\mathbf{K}}_{ij}^{(k)})_{mn} = \int_{\Omega^{(k)}} \eta_{m,i}^{\mathcal{N}} \eta_{n,j}^{\mathcal{N}} dx \ .$$

In the online stage, we first form a parameter-dependent matrix $\mathbf{K}(\mu) \in \mathbb{R}^{N\times N}$ defined by

$$\mathbf{K}(\mu) \equiv \sum_{k=1}^{K_{\rm dom}} \sum_{i,j=1}^{d} (D^{(k)}(\mu))_{ij}^{-1} \hat{\mathbf{K}}_{ij}^{(k)}.$$

We then solve the $N \times N$ quadratic program with the single linear constraint and form the lower bound as before. The computational complexity in the online stage is $\mathcal{O}(K_{\rm dom} d^2 N^2) + \mathcal{O}((N+1)^3)$.

3.3. Extension 3: Reaction-Diffusion Equation

We now consider an extension of the method to the reaction-diffusion equation. The bilinear form associated with the equation is

$$a(w,v;\mu) \equiv \int_\Omega \left(\nabla v \cdot D(\mu)\nabla w + c(\mu) v w\right) dx$$

and the associated energy functional is $\mathcal{J}_p(w;\mu) \equiv \frac{1}{2}a(w,w;\mu) - \ell(w)$. The solution $u(\mu) \in V$ such that $a(u,v;\mu) = \ell(v)$, $\forall v \in V$, is the infimizer of the energy functional. Thus, owing to the variational structure, the construction of an upper bound requires no modifications.

To construct a lower bound, we first introduce the second dual variable $z \in \hat{V}$, where we recall $\hat{V}$ is the broken space defined in (1). We then redefine the bilinear form that induces the dual feasibility constraint:

$$b((q,z),w) \equiv \int_\Omega \left(q\cdot\nabla w + z w\right) dx, \quad \forall q \in \hat{Y},\ \forall z \in \hat{V},\ \forall w \in V \ .$$

We next redefine the dual feasible space

$$Q \equiv \{(q,z) \in \hat{Y} \times \hat{V} : b((q,z),w) = \ell(w),\ \forall w \in V\}\ .$$

We finally introduce the dual energy functional

$$\mathcal{J}_d((q,z);\mu) \equiv -\frac{1}{2}\int_\Omega \left(q \cdot D^{-1}(\mu) q + c^{-1}(\mu) z z\right) dx, \quad \forall q \in \hat{Y},\ \forall z \in \hat{V}\ .$$

We may then show

$$J(\mu) \geq \mathcal{J}_d((q,z);\mu), \quad \forall (q,z) \in Q\ ,$$

following the same argument as the proof of Proposition 1.

In order to construct a finite element approximation of the dual variables $(q,z) \in Q$, we follow the same localization procedure. (See Sauer-Budge and Peraire [17] for details.) Namely, we first compute the equilibrating inter elemental flux $\lambda^{\mathcal{N}}(\mu) \in \Lambda$ as defined by (7) (for the $a(\cdot,\cdot;\mu)$ associated with the reaction-diffusion equation). We then identify the strong form of the local constraints

$$\begin{aligned} -\nabla \cdot q + z &= f \quad \text{in } H^{-1}(\kappa), \quad \forall \kappa \in \mathcal{T}_h\ , \\ \hat{n}_\kappa \cdot q &= \sigma_\kappa \lambda^{\mathcal{N}}(\mu) \quad \text{in } H^{-1/2}(\partial\kappa), \quad \forall \kappa \in \mathcal{T}_h\ . \end{aligned}$$

Here, for $f|_\kappa \in \mathbb{P}^{p_f}(\kappa)$, $\lambda^{\mathcal{N}}(\mu)|_\gamma \in \mathbb{P}^p(\gamma)$, $\forall \gamma \in \partial\kappa$, and $p > p_f$, we may choose $q|_\kappa \in \mathbb{P}^p(\kappa)$ and $z|_\kappa \in \mathbb{P}^{p-1}(\kappa)$; we then realize, as before, we need only test the equation over κ against $\mathbb{P}^{p-1}(\kappa)$ and the equations over $\partial\kappa$ against $\mathbb{P}^p(\gamma)$, $\gamma \in \partial\kappa$. Thus, we can express the dual feasibility condition as a finite dimensional constraints. The existence of at least one solution $(q,z) \in \hat{Y}^{\mathcal{N}} \times \hat{V}^{\mathcal{N}}$ that satisfies the dual feasibility conditions, and hence the non-emptiness of $\hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu))$, is a consequence of the existence condition for the diffusion equation; the presence of the dual variable associated with the reaction term, $z \in \hat{V}^{\mathcal{N}}$, increases the number of unknowns while the number of constrains is unchanged. We then seek $(p^{\mathcal{N}}(\mu), r^{\mathcal{N}}(\mu)) \equiv \arg\sup_{(q^{\mathcal{N}},z^{\mathcal{N}}) \in \hat{Q}^{\mathcal{N}}(\lambda^{\mathcal{N}}(\mu))} \mathcal{J}_d((q^{\mathcal{N}},z^{\mathcal{N}});\mu)$.

We now deduce the constraints in the reduced basis setting. We first introduce an orthonormalized basis of the reduced basis space $\hat{Y}_N$, $\{(\eta_n^{\mathcal{N}}, \zeta_n^{\mathcal{N}})\}_{n=1}^N$; the change of basis matrix $\omega \in \mathbb{R}^{N\times N}$ satisfies

$$(\eta_n^{\mathcal{N}}, \zeta_n^{\mathcal{N}}) = \left(\sum_{n'=1}^N p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n},\ \sum_{n'=1}^N r^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\right).$$

We express our reduced basis approximation as $p_N = \sum_{n=1}^N \eta_n^{\mathcal{N}} \beta_{Nn} = \sum_{n=1}^N \sum_{n'=1}^N p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}$ and $r_N = \sum_{n=1}^N \zeta_n^{\mathcal{N}} \beta_{Nn} = \sum_{n=1}^N \sum_{n'=1}^N r^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}$, appeal to the bilinearity of $b(\cdot,\cdot)$, and $(p^{\mathcal{N}}(\mu_{(n')}), r^{\mathcal{N}}(\mu_{(n')})) \in Q$ — which implies $b((p^{\mathcal{N}}(\mu_{(n')}), r^{\mathcal{N}}(\mu_{(n')})), w) = \ell(w)$, $\forall w \in V$, $n' = 1, \ldots, N$ — to obtain

$$\begin{aligned} b((p_N, r_N), w) &= b((\sum_{n=1}^N \sum_{n'=1}^N p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}, \sum_{n=1}^N \sum_{n'=1}^N r^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}), w) \\ &= \sum_{n=1}^N \sum_{n'=1}^N \omega_{n'n}\beta_{Nn} b((p^{\mathcal{N}}(\mu_{(n')}), r^{\mathcal{N}}(\mu_{(n')})), w) \\ &= \sum_{n=1}^N \sum_{n'=1}^N \omega_{n'n}\beta_{Nn} \ell(w), \quad \forall w \in V\ ; \end{aligned}$$

we recognize the sufficient condition for $p_N(\mu) \in Q$ is $\sum_{n=1}^N \sum_{n'=1}^N \omega_{n'n}\beta_{Nn} = 1$ — the same condition as the diffusion-only case.

The offline-online computational decomposition is similar to the diffusion-only case. In the offline stage, we first solve N finite element dual problems to obtain basis functions $p^{\mathcal{N}}(\mu_{(n')})$ and $r^{\mathcal{N}}(\mu_{(n')})$, $n' = 1, \ldots, N$. We then orthonormalize the functions to obtain $\eta_n^{\mathcal{N}}$ and $\zeta_n^{\mathcal{N}}$, $n = 1, \ldots, N$, and the change of basis matrix $\omega \in \mathbb{R}^{N\times N}$. We next sum the leading index of the change of basis matrix to form $\omega_n^{\text{sum}} = \sum_{n'=1}^N \omega_{n'n}$. We then compute parameter-independent matrices $\hat{\mathbf{K}}_{ij} \in \mathbb{R}^{N\times N}$, $i, j = 1, \ldots, d$ and $\hat{\mathbf{C}} \in \mathbb{R}$, with entries

$$(\hat{\mathbf{K}}_{ij})_{mn} = \int_\Omega \eta_{m,i}^{\mathcal{N}} \eta_{n,j}^{\mathcal{N}} dx \quad \text{and} \quad \hat{\mathbf{C}}_{mn} = \int_\Omega \zeta_m^{\mathcal{N}} \zeta_n^{\mathcal{N}} dx \ .$$

In the online stage, we take a three-step procedure as before. We first form parameter-dependent matrices $\mathbf{K}(\mu) \in \mathbb{R}^{N\times N}$ and $\mathbf{C}(\mu) \in \mathbb{R}^{N\times N}$ defined by

$$\mathbf{K}(\mu) \equiv \sum_{i,j=1}^d D_{ij}^{-1}(\mu)\hat{\mathbf{K}}_{ij} \quad \text{and} \quad \mathbf{C}(\mu) \equiv c^{-1}(\mu)\hat{\mathbf{C}} \ .$$

We then solve a $N \times N$ quadratic program with a single linear constraint

$$\beta_N^\star(\mu) = \underset{\substack{\beta_N \in \mathbb{R}^N \\ (\omega^{\text{sum}})^T\beta_N = 1}}{\arg\sup} \ -\frac{1}{2}\beta_N^T(\mathbf{K}(\mu) + \mathbf{C}(\mu))\beta_N \ ,$$

which requires the solution of a $(N + 1) \times (N + 1)$ saddle system. We finally evaluate the lower bound

$$J_N^-(\mu) = -\frac{1}{2}(\beta_N^\star(\mu))^T(\mathbf{K}(\mu) + \mathbf{C}(\mu))\beta_N^\star(\mu) \ .$$

The computational complexity in the online stage is $\mathcal{O}(d^2N^2) + \mathcal{O}((N + 1)^3)$.

Remark 3. We have here used the same reduced basis coefficients, β_N, for $p_N = \sum_{n=1}^N \eta_n^{\mathcal{N}}\beta_{Nn}$ and $r_N = \sum_{n=1}^N \zeta_n^{\mathcal{N}}\beta_{Nn}$. We may instead consider different coefficients for the two spaces. The coupled formulation, as considered in this work, is typically more online efficient as $p(\mu)$ and $r(\mu)$ tend to be correlated. The decoupled formulation is less online efficient but is more offline efficient: it produces an online system of size $2N$, but the reduced basis space has a larger dimension for a given number of offline snapshots.

3.4. Extension 4: Affine Geometry Transformation (Reaction-Diffusion)

We now consider an application of the method to problems with an affine geometry transformation. By way of preliminaries, we introduce a parameter-independent reference domain $\tilde{\Omega}$ and a parameter-dependent transformed domain $\Omega(\mu)$. A point $\tilde{x} \in \tilde{\Omega}$ is mapped to a point $x \in \Omega(\mu)$ by an affine transformation

$$x = G(\tilde{x}; \mu) \equiv T(\mu)\tilde{x} + x_0(\mu),$$

where $T(\mu) \in \mathbb{R}^{d\times d}$ is the Jacobian of the transformation, and $x_0(\mu) \in \mathbb{R}^d$ is associated with the translation.

We may readily transform the forms associated with the parameter-dependent domain $\Omega(\mu)$ to the forms associated with the parameter-independent reference domain $\tilde{\Omega}$. (We refer to Rozza *et al.* [15] for more detailed discussion in the standard reduced basis context.) We first transform the bilinear form $a(\cdot,\cdot;\mu)$: for $\tilde{w} = w \circ G(\cdot;\mu)$ and $\tilde{v} = v \circ G(\cdot;\mu)$,

$$a(w,v;\mu) \equiv \int_{\Omega(\mu)} [\nabla v \cdot D(\mu) \nabla w + c(\mu) v w]\, dx = \int_{\tilde{\Omega}} \left[\tilde{\nabla}\tilde{v} \cdot \tilde{D}(\mu)\tilde{\nabla}\tilde{w} + \tilde{c}(\mu)\tilde{w}\tilde{v}\right] d\tilde{x} \equiv \tilde{a}(\tilde{w},\tilde{v};\mu),$$

where $\tilde{D}(\mu) \equiv \det(T(\mu)) T^{-T}(\mu) D(\mu) T^{-1}(\mu)$ and $\tilde{c}(\mu) \equiv \det(T(\mu)) c(\mu)$. We then transform the linear form $\ell(\cdot;\mu)$: for $\tilde{v} = v \circ G(\cdot;\mu)$,

$$\ell(v;\mu) \equiv \int_{\Omega(\mu)} f(\mu) v dx + \int_{\Gamma_N(\mu)} g(\mu) v ds = \int_{\tilde{\Omega}} \tilde{f}(\mu)\tilde{v} d\tilde{x} + \int_{\tilde{\Gamma}_N} \tilde{g}(\mu)\tilde{v} d\tilde{s} \equiv \tilde{\ell}(\tilde{v};\mu),$$

where $\tilde{f}(\mu) \equiv (\det(T(\mu)) f(\mu)) \circ G(\cdot;\mu)$ and $\tilde{g}(\mu) \equiv (\det(T_{\Gamma_N}(\mu)) g(\mu)) \circ G(\cdot;\mu)$. We in addition define the primal energy functional on the reference domain: $\tilde{\mathcal{J}}_p(\cdot;\mu) \equiv \frac{1}{2}\tilde{a}(\cdot,\cdot;\mu) - \tilde{\ell}(\cdot;\mu)$. The transformation for $a(\cdot,\cdot;\mu)$ and $\ell(\cdot;\mu)$ are in fact the standard transformation in the reduced basis context [15].

We now introduce a key transformation for the lower bound construction. We transform the bilinear form $b(\cdot,\cdot;\mu)$, which is now parameter *dependent* due to the presence of $\Omega(\mu)$, as follows: for $\tilde{q} \equiv (\det(T(\mu)) T^{-T}(\mu) q) \circ G(\cdot;\mu)$, $\tilde{z} \equiv (\det(T(\mu)) z) \circ G(\cdot;\mu)$, and $\tilde{w} = w \circ G(\cdot;\mu)$,

$$\begin{aligned} b((q,z),w;\mu) &\equiv \int_{\Omega(\mu)} (q \cdot \nabla w + z w)\, dx = \int_{\tilde{\Omega}} \left(q \cdot T^{-1}(\mu)\tilde{\nabla}\tilde{w} \det(T(\mu)) + z\tilde{w}\det(T(\mu))\right) d\tilde{x} \\ &= \int_{\tilde{\Omega}} \left(\tilde{q} \cdot \tilde{\nabla}\tilde{w} + \tilde{z}\tilde{w}\right) d\tilde{x} \equiv \tilde{b}((\tilde{q},\tilde{z}),\tilde{w}). \end{aligned}$$

We note that the transformed bilinear form $\tilde{b}(\cdot,\cdot)$ is in fact *independent* of the parameter μ. Accordingly, we may identify the space of dual feasible functions in the reference domain

$$Q(\tilde{\Omega};\mu) \equiv \{(\tilde{q},\tilde{z}) \in \hat{Y}(\tilde{\Omega}) \times \hat{V}(\tilde{\Omega}) : \tilde{b}((\tilde{q},\tilde{z}),\tilde{w}) = \tilde{\ell}(\tilde{w};\mu),\ \forall \tilde{w} \in V(\tilde{\Omega})\}, \tag{15}$$

where the parameter-dependence of the dual-feasibility condition arises only through the right-hand side, $\tilde{\ell}$, and can be treated using the technique in Section 3.1. We readily confirm that, if $(\tilde{q},\tilde{z}) \in Q(\tilde{\Omega};\mu)$, then $(q,z) \equiv (((\det(T(\mu)))^{-1} T^T(\mu)\tilde{q}) \circ G^{-1}(\cdot,\mu), ((\det(T(\mu)))^{-1}\tilde{z}) \circ G^{-1}(\cdot,\mu)) \in Q(\Omega;\mu)$ for $Q(\Omega;\mu) \equiv \{(q,z) \in \hat{Y}(\Omega(\mu)) \times \hat{V}(\Omega(\mu)) : b((q,z),w;\mu) = \ell(w;\mu),\ \forall w \in V(\Omega(\mu))\}$. We in addition note that the dual energy functional admits the following transformation: for $\tilde{q} \equiv (\det(T(\mu)) T^{-T}(\mu) q) \circ G(\cdot;\mu)$ and $\tilde{z} \equiv (\det(T(\mu)) z) \circ G(\cdot;\mu)$,

$$\begin{aligned} \mathcal{J}_d((q,z);\mu) &\equiv -\frac{1}{2} \int_{\Omega(\mu)} \left(q \cdot D^{-1}(\mu) q + c^{-1}(\mu) z z\right) dx \\ &= -\frac{1}{2} \int_{\tilde{\Omega}} \left(\tilde{q} \cdot \tilde{D}^{-1}(\mu)\tilde{q} + \tilde{c}^{-1}\tilde{z}\tilde{z}\right) d\tilde{x} \equiv \tilde{\mathcal{J}}_d((\tilde{q},\tilde{z});\mu), \end{aligned}$$

where $\tilde{D}(\mu)$ and $\tilde{c}(\mu)$ are as defined for $\tilde{a}(\cdot,\cdot;\mu)$.

We summarize the computational strategy. We first recast the primal and dual problems on $\Omega(\mu)$ as those on the reference domain $\tilde{\Omega}$; we identify the associated forms $\tilde{a}(\cdot,\cdot;\mu)$, $\tilde{\ell}(\cdot;\mu)$, $\tilde{\mathcal{J}}_p(\cdot;\mu)$, $\tilde{b}(\cdot,\cdot)$, and $\tilde{\mathcal{J}}_d(\cdot;\mu)$. We then apply the method developed in Section 2 (with the extensions introduced in Sections 3.1 and 3.3) in the reference domain $\tilde{\Omega}$ to construct the bounds $J_N^+(\mu)$ and $J_N^-(\mu)$.

3.5. Extension 5: Linear Elasticity

We now consider an extension of the method to linear elasticity. For clarity in this section, we employ the index notation with the implied summation on repeated indices. We first introduce a space of vector-valued functions

$$V \equiv \{v \in (H^1(\Omega))^d : v_i|_{\Gamma_{D,i}} = 0,\ i = 1, \ldots, d\},$$

where $\Gamma_{D,i}$ is the boundary with the homogeneous Dirichlet condition on the i-th equation. The bilinear form is

$$a(w, v; \mu) \equiv \int_\Omega \epsilon_{ki}(v) C_{kilj}(\mu) \epsilon_{lj}(w) dx;$$

here $\epsilon(v) \in (L^2(\Omega))^{d\times d}$ is the strain tensor given by $\epsilon_{ij}(v) \equiv \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$, and $C(\mu)$ is the rank-four stiffness tensor. The linear form is

$$\ell(w) = \int_\Omega f_k v_k dx + \int_{\Gamma_N} g_k v_k dx,$$

where $f \in (L^2(\Omega))^d$ specifies the body force, and $g \in \otimes_{i=1}^d L^2(\Gamma_{N,i})$ specifies the traction on boundaries. The associated energy functional is $\mathcal{J}_p(w; \mu) \equiv \frac{1}{2} a(w, w; \mu) - \ell(w)$. Again, owing to the variational structure of the problem, the construction of an upper bound is straightforward.

To construct a lower bound, we first introduce a broken space of vector-valued functions $\hat{V}$ associated with V and a space of rank-two tensor-valued functions $\hat{Y} \equiv (\hat{V})^d$. We then redefine the bilinear form

$$b(q, w) \equiv \int_\Omega q_{ki} \epsilon_{ki}(w) dx, \quad \forall q \in \hat{Y},\ \forall w \in V\ .$$

We next redefine the dual feasible space

$$Q \equiv \{q \in \hat{Y} : b(q, w) = \ell(w),\ \forall w \in V\}.$$

We finally redefine the dual energy functional

$$\mathcal{J}_d(q; \mu) \equiv -\frac{1}{2} \int_\Omega q_{ki} C^{-1}_{kilj}(\mu) q_{lj} dx, \quad \forall q \in \hat{Y}\ .$$

We may then show that $J(\mu) \geq \mathcal{J}_d(q; \mu)$, $\forall q \in Q$, following a vectorized version of the proof of Proposition 1.

In order to construct a finite element approximation of the dual variable, we follow the procedure of Pares *et al.* [10]. We first extend the definition of the trace space Λ to vector-valued functions (in the same manner as V). We accordingly refine the bilinear forms $\hat{c}(\cdot, \cdot)$ and $\hat{b}(\cdot, \cdot)$ as

$$\hat{c}(\hat{w}, \chi) \equiv \sum_{\kappa \in \mathcal{T}_h} \int_{\partial\kappa} \sigma_\kappa \hat{w}_k \chi_k ds, \quad \forall \hat{w} \in \hat{V},\ \forall \chi \in \Lambda$$

$$\hat{b}(q, \hat{w}) \equiv \sum_{\kappa \in \mathcal{T}_h} \int_\kappa q_{ki} \epsilon_{ki}(w) dx, \quad \forall q \in \hat{Y},\ \forall \hat{w} \in \hat{V}\ .$$

We may readily compute the vector-valued equilibrating inter elemental flux, $\lambda^{\mathcal{N}}(\mu) \in \Lambda$, as defined by (7). On the other hand, the construction of the dual feasible functions via the localization is more complicated than for the diffusion equation, not because it is a vector equation, but because the map from the space of gradients to the strain is not bijective. Nevertheless, a *piecewise* $\mathbb{P}^p$ polynomial representation of a function in Q over each $\kappa \in \mathcal{T}_h$ may be found, for any $f|_\kappa \in (\mathbb{P}^{p_f}(\kappa))^d$, $g|_\gamma \in (\mathbb{P}^{p_f}(\gamma))^d$, and $\lambda|_\gamma \in (\mathbb{P}^p(\gamma))^d$, $\forall \gamma \in \partial\kappa$, using a subgrid computation procedure described by Pares *et al.* [10]; we omit the presentation of the procedure for brevity. (See also Pled *et al.* [12] for alternative strategies.)

While the finite element approximation of the dual variable is more complicated, the reduced basis approximation requires only minor modifications from the diffusion equation case considered in Section 2. This is because, for $p_N = \sum_{n=1}^N \sum_{n'=1}^N p^{\mathcal{N}}(\mu_{(n')})\omega_{n'n}\beta_{Nn}$, the condition for $p_N \in Q$ is $\sum_{n=1}^N \sum_{n'=1}^N \omega_{n'n}\beta_{Nn} = 1$ as before.

In the offline stage, we first compute snapshots $p^{\mathcal{N}}(\mu_{(n')}) \in Q$, $n' = 1, \ldots, N$. We then orthonormalize the functions to form the basis $\{\eta_n^{\mathcal{N}}\}_{n=1}^N$ for the reduced basis space $\hat{Y}_N$ and the change of basis matrix $\omega \in \mathbb{R}^{N\times N}$. We next sum the leading index of the change of basis matrix to form $\omega_n^{\text{sum}} = \sum_{n'=1}^N \omega_{n'n}$. We then compute parameter-independent matrices $\hat{\mathbf{K}}_{ijkl} \in \mathbb{R}^{N\times N}$, $i, j, k, l = 1, \ldots, d$, with entries

$$(\hat{\mathbf{K}}_{kilj})_{mn} = \int_\Omega \eta_{m,ki}^{\mathcal{N}} \eta_{n,lj}^{\mathcal{N}} dx \ ;$$

here $\eta_{m,ki}$ denotes the (k, i) tensor-entry of the m-th basis function. In the online stage, we first form a parameter-dependent matrix $\mathbf{K}(\mu) \in \mathbb{R}^{N\times N}$ defined by

$$\mathbf{K}(\mu) \equiv \sum_{k,i,l,j=1}^{d} C_{kilj}^{-1}(\mu)\hat{\mathbf{K}}_{kilj};$$

we then solve a quadratic program

$$J_N^-(\mu) \equiv \sup_{q_N \in Q_N} \mathcal{J}_d(q_N; \mu) = \sup_{\substack{q_N \in \hat{Y}_N \\ (\omega^{\text{sum}})^T \beta_N = 1}} \mathcal{J}_d(q_N; \mu)$$

with a single linear constraint and form the lower bound as before. The computational complexity in the online stage is $\mathcal{O}(d^4 N^2) + \mathcal{O}((N+1)^3)$.

3.6. Extension 6: Affine Geometry Transformation (Linear Elasticity)

We now consider an application of the method to linear elasticity problems with affine geometry mapping. The strategy is similar to that for the reaction-diffusion equation presented in Section 3.4; however, we must now transform the vector-valued primal variable and rank-two tensor-valued dual variable in a consistent manner. As before, the transformation from the parameter-independent reference domain $\tilde{\Omega}$ to the parameter-dependent transformed domain $\Omega(\mu)$ is denoted by $x = G(\tilde{x}; \mu) \equiv T(\mu)\tilde{x} + x_0(\mu)$. To avoid the notational clutter, we simply state $T(\mu)$ as T from hereon.

We first note the transformation of the strain tensor: for $\tilde{w}_k = (T_{lk} w_l) \circ G(\cdot; \mu)$, $\epsilon_{ij}(w) = T_{ki}^{-1} T_{lj}^{-1} \tilde{\epsilon}_{kl}(\tilde{w})$ where $\tilde{\epsilon}_{kl}(\tilde{w}) \equiv \frac{1}{2}\left(\frac{\partial \tilde{w}_k}{\partial \tilde{x}_l} + \frac{\partial \tilde{w}_l}{\partial \tilde{x}_k}\right)$. We next transform the bilinear form $a(\cdot, \cdot; \mu)$: for $\tilde{w}_k = (T_{lk} w_l) \circ G(\cdot; \mu)$ and $\tilde{v}_k = (T_{lk} v_l) \circ G(\cdot; \mu)$,

$$a(w, v; \mu) \equiv \int_{\Omega(\mu)} \epsilon_{ki}(v) C_{kilj}(\mu) \epsilon_{lj}(w) dx = \int_{\tilde{\Omega}} \tilde{\epsilon}_{ki}(\tilde{v}) \tilde{C}_{kilj} \tilde{\epsilon}_{lj}(\tilde{w}) d\tilde{x} \equiv \tilde{a}(\tilde{w}, \tilde{v}; \mu),$$

where $\tilde{C}_{kilj}(\mu) \equiv \det(T) T^{-1}_{sk} T^{-1}_{mi} T^{-1}_{tl} T^{-1}_{nj} C_{smtn}(\mu)$. We then transform the linear form: for $\tilde{v}_k = (T_{lk} v_l) \circ G(\cdot;\mu)$,

$$\ell(w) \equiv \int_{\Omega(\mu)} f_k v_k dx + \int_{\Gamma_N} g_k v_k ds = \int_{\tilde{\Omega}} \tilde{f}_k \tilde{v}_k d\tilde{x} + \int_{\tilde{\Gamma}_N} \tilde{g}_k \tilde{v}_k d\tilde{s} \equiv \int_{\tilde{\Omega}} (\tilde{w}),$$

where $\tilde{f}_k(\mu) = (\det(T) T^{-1}_{kl} f_l(\mu)) \circ G(\cdot;\mu)$ and $\tilde{g}_k(\mu) = (\det(T_{\Gamma_N}) T^{-1}_{kl} g_l(\mu)) \circ G(\cdot;\mu)$. We in addition define the primal energy functional on the reference domain: $\tilde{\mathcal{J}}_p(\cdot;\mu) \equiv \frac{1}{2}\tilde{a}(\cdot,\cdot;\mu) - \tilde{\ell}(\cdot;\mu)$.

We now consider transformations associated with the lower bound construction. We transform the bilinear form $b(\cdot,\cdot;\mu)$, which again is parameter dependent due to the presence of $\Omega(\mu)$, as follows: for $\tilde{q}_{kl} = (\det(T) T^{-1}_{ki} T^{-1}_{lj} q_{ij}) \circ G(\cdot;\mu)$

$$b(q, w; \mu) \equiv \int_{\Omega(\mu)} q_{ki} \epsilon_{ki}(w) dx = \int_{\tilde{\Omega}} \tilde{q}_{ki} \tilde{\epsilon}_{ki}(\tilde{w}) d\tilde{x} \equiv \tilde{b}(\tilde{q}, \tilde{w}).$$

We again note that the transformed bilinear form $\tilde{b}(\cdot,\cdot)$ is independent of the parameter μ. We then introduce the space of dual feasible functions on the reference domain $Q(\tilde{\Omega};\mu) \equiv \{\tilde{q} \in \hat{Y}(\tilde{\Omega}) : \tilde{b}(\tilde{q},\tilde{w}) = \tilde{\ell}(\tilde{w};\mu),\ \forall \tilde{w} \in V(\tilde{\Omega})\}$. We readily confirm that, if $\tilde{q}(\mu) \in Q(\tilde{\Omega};\mu)$, then $q_{kl} \equiv ((\det(T))^{-1} T_{ki} T_{lj} \tilde{q}_{ij}) \circ G^{-1}(\cdot,\mu) \in Q(\Omega;\mu)$ for $Q(\Omega;\mu) \equiv \{q \in \hat{Y}(\Omega(\mu)) : b(q,w;\mu) = \ell(w;\mu),\ \forall w \in V(\Omega(\mu))\}$. Finally, we note that the dual energy functional admits the following transformation: for $\tilde{q}_{kl} = (\det(T) T^{-1}_{ki} T^{-1}_{lj} q_{ij}) \circ G(\cdot;\mu)$,

$$\mathcal{J}_d(q;\mu) \equiv -\frac{1}{2} \int_{\Omega(\mu)} q_{ki} C^{-1}_{kilj}(\mu) q_{lj} dx = -\frac{1}{2} \int_{\tilde{\Omega}} \tilde{q}_{ki} \tilde{C}^{-1}_{kilj}(\mu) \tilde{q}_{lj} d\tilde{x} \equiv \mathcal{J}_d(\tilde{q};\mu),$$

where $\tilde{C}$ is as defined for $\tilde{a}(\cdot,\cdot;\mu)$.

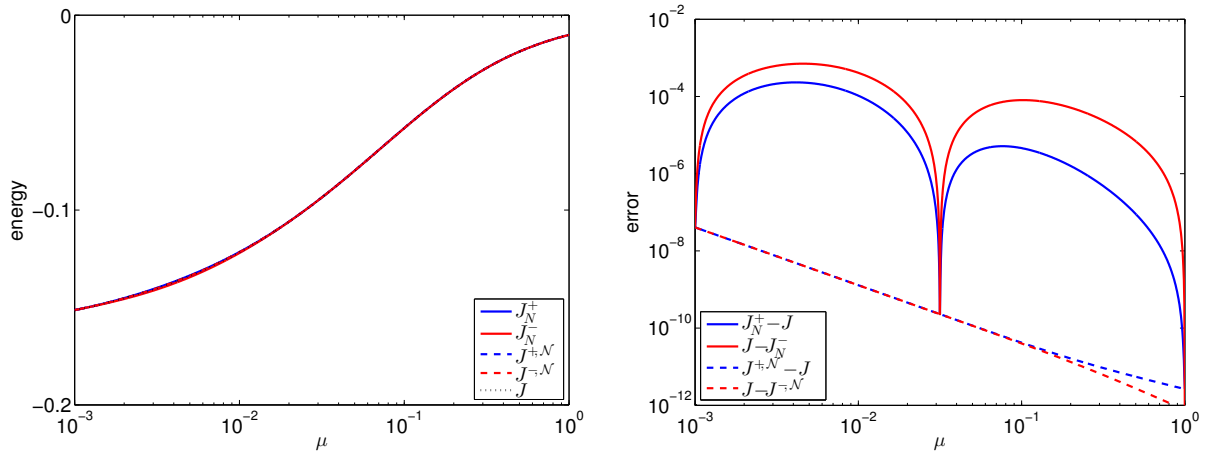
The computational strategy follows that of the reaction-diffusion case in Section 3.4. We first recast the primal and dual problems on $\Omega(\mu)$ to those on the reference domain $\tilde{\Omega}$; we identify the associated forms $\tilde{a}(\cdot,\cdot;\mu)$, $\tilde{\ell}(\cdot;\mu)$, $\tilde{\mathcal{J}}_p(\cdot;\mu)$, $\tilde{b}(\cdot,\cdot)$, and $\tilde{\mathcal{J}}_d(\cdot;\mu)$. We then apply the method developed in Section 2 (with the extensions introduced in Sections 3.1 and 3.5) in the reference domain $\tilde{\Omega}$ to construct the bounds $J^+_N(\mu)$ and $J^-_N(\mu)$.

4. Results

4.1. One-Dimensional Reaction-Diffusion Equation

We first apply the exact certification technique to a parametrized reaction-diffusion equation: $-\mu\Delta u + u = x$ over $\Omega \equiv (0,1)$ with homogeneous Dirichlet boundary conditions at $x = 0$ and $x = 1$. The diffusion coefficient takes on $\mu \in \mathcal{D} \equiv [10^{-3}, 1]$. Our finite element spaces consist of n_e equal-sized $\mathbb{P}^2$ elements ($\mathcal{N} = 2n_e - 1$). Our reduced basis space is constructed from the finite element solution evaluated at N Chebyshev-Lobatto nodes of $\mathcal{D}$ mapped by a logarithmic transformation [9]. The exact energy $J(\mu)$ is computed using a $\mathbb{P}^{30}$ pseudo-spectral discretization. Our reduced basis formulation exercises the extension considered in Sections 3.3.

The bound behavior for the $n_e = 128$, $N = 3$ case is shown in Figure 1. The $\mathbb{P}^2$ finite element discretization with $n_e = 128$ elements is sufficient to obtain the maximum error over the parameter range of $\mathcal{O}(10^{-8})$; hence, this is the typically assumed reduced basis scenario where the finite element discretization may be taken as the "truth." As a result, the error plot over the parameter



(a) energy (b) error

Figure 1: The behavior of the bounds for the reaction-diffusion problem for $n_e = 128$ and $N = 3$. (J: truth; $J_N^{\pm}$: reduced basis bounds; $J^{\pm,\mathcal{N}}$: finite element bounds)

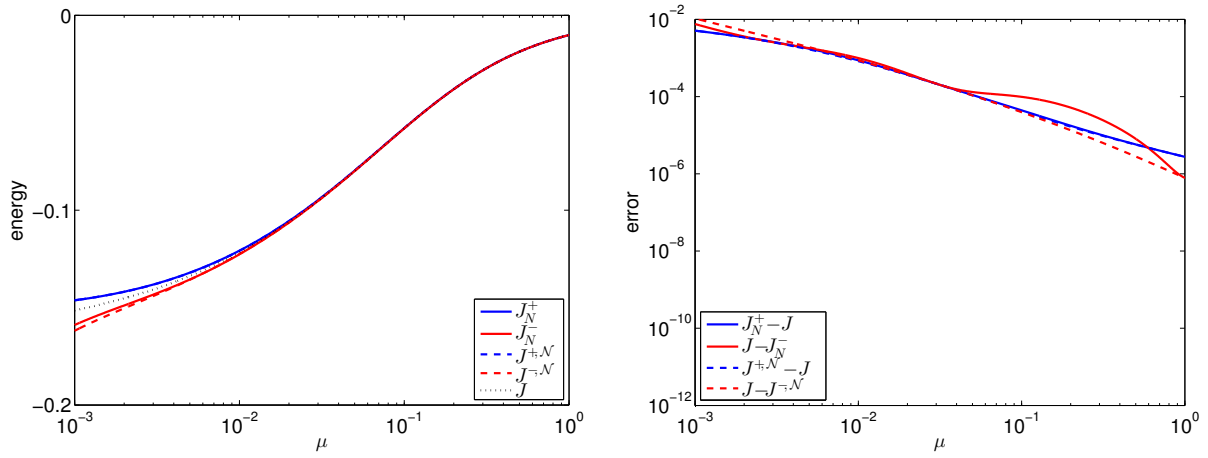
domain exhibits the typical reduced basis method error behavior; namely, the error essentially vanishes at the reduced basis parameter evaluation points and grows away from the points.

The bound behavior for the $n_e = 4$, $N = 3$ case is shown in Figure 2. The $\mathbb{P}^2$, $n_e = 4$ finite element discretization provides insufficient resolution particularly for a small μ; this is reflected in the noticeable finite element bound gap. The quality of the reduced basis bound is limited by the inadequacy of the underlying finite element discretization.

Table 1 summarizes the maximum error of the reduced basis bound over $\Xi \subset \mathcal{D}$, where the surrogate subset Ξ consists of 1001 points equidistributed over $\mathcal{D}$ in the logarithmic sense. The error in the bound is expressed as a function of the physical space resolution (as reflected in n_e) and the parameter space resolution (as reflected in N). We first report that the upper and lower bounds are indeed rigorous bounds of the exact energy $J(\mu)$: $J_N^+(\mu) - J(\mu) > 0$ and $J - J_N^-(\mu) > 0$ for all $\mu \in \mathcal{D}$, n_e, and N. We next comment on the two extreme cases shown in the table: for $n_e = 4$, the physical space resolution limits the bound quality independent of the parameter space resolution; for $N = 1$, the parameter space resolution limits the bound quality independent of the physical space resolution. We also note that the finite element bounds converge at the optimal rate of $h^{2p} = h^4$ for this smooth problem. Finally, given a sufficient finite element resolution (for instance for $n_e = 128$), the reduced basis bounds exhibit an exponential convergence with N.

4.2. Planar Linear Elasticity

We now consider a planar (stress) elasticity problem with a geometry deformation; we refer to, for instance, Rozza *et al.* [15] for the treatment of linear elasticity problems in the standard reduced basis context. We consider an rectangular elastic beam of a length (normalized with respect to the height) of $L/H \in [2.0, 8.0]$ composed of a material with a (non-dimensionalized) Young's modulus 1.0 and Poisson's ratio of 0.3. The beam is fully clamped on one end, and we apply an unit tangential traction on the other end; all other boundaries are traction free. We then compute upper and lower bounds of the elastic energy as the length is varied; recall that, by Proposition 3, the energy bound gap may be used to construct a bound of the energy norm of the field. Our finite element spaces consist of $\mathbb{P}^3$ elements on a sequence of uniformly refined



(a) energy (b) error

Figure 2: The behavior of the bounds for the reaction-diffusion problem for $n_e = 4$ and $N = 3$. (J: truth; $J_N^{\pm}$: reduced basis bounds; $J^{\pm,\mathcal{N}}$: finite element bounds)

(a) upper bound error: $\max_{\mu\in\Xi\subset\mathcal{D}}(J_N^+(\mu) - J(\mu))$

	$n_e = 4$	8	16	32	64	128
$N = 1$	1.90×10^{-2}	1.84×10^{-2}	1.83×10^{-2}	1.83×10^{-2}	1.83×10^{-2}	1.83×10^{-2}
2	5.10×10^{-3}	2.69×10^{-3}	3.16×10^{-3}	3.26×10^{-3}	3.27×10^{-3}	3.27×10^{-3}
3	5.10×10^{-3}	1.01×10^{-3}	2.30×10^{-4}	2.31×10^{-4}	2.32×10^{-4}	2.32×10^{-4}
4	5.10×10^{-3}	1.01×10^{-3}	1.20×10^{-4}	1.10×10^{-5}	7.83×10^{-6}	7.64×10^{-6}
5	5.10×10^{-3}	1.01×10^{-3}	1.20×10^{-4}	9.54×10^{-6}	6.39×10^{-7}	4.39×10^{-7}
6	5.10×10^{-3}	1.01×10^{-3}	1.20×10^{-4}	9.54×10^{-6}	6.39×10^{-7}	4.07×10^{-8}
FE	5.10×10^{-3}	1.01×10^{-3}	1.20×10^{-4}	9.54×10^{-6}	6.39×10^{-7}	4.07×10^{-8}

(b) lower bound error: $\max_{\mu\in\Xi\subset\mathcal{D}}(J(\mu) - J_N^-(\mu))$

	$n_e = 4$	8	16	32	64	128
$N = 1$	8.36×10^{-1}	8.21×10^{-1}	8.20×10^{-1}	8.20×10^{-1}	8.20×10^{-1}	8.20×10^{-1}
2	9.39×10^{-3}	9.51×10^{-3}	1.01×10^{-2}	1.02×10^{-2}	1.02×10^{-2}	1.02×10^{-2}
3	7.58×10^{-3}	1.11×10^{-3}	6.95×10^{-4}	7.04×10^{-4}	7.06×10^{-4}	7.06×10^{-4}
4	6.17×10^{-3}	1.06×10^{-3}	1.21×10^{-4}	2.84×10^{-5}	2.84×10^{-5}	2.84×10^{-5}
5	5.66×10^{-3}	1.02×10^{-3}	1.20×10^{-4}	9.54×10^{-6}	2.20×10^{-6}	2.18×10^{-6}
6	5.32×10^{-3}	1.01×10^{-3}	1.20×10^{-4}	9.54×10^{-6}	6.39×10^{-7}	1.00×10^{-7}
FE	1.06×10^{-2}	1.21×10^{-3}	1.23×10^{-4}	9.55×10^{-6}	6.39×10^{-7}	4.07×10^{-8}

Table 1: Convergence of the reduced basis upper and lower energy bounds (and the finite element bounds) for the reaction-diffusion problem with the number of elements in the underlying $\mathbb{P}^2$ finite element discretization (n_e) and the reduced basis space dimension (N).

	$\mathcal{N} = 175$	637	2,425	9,457	37,345	148,417
$N = 1$	9.95×10^{-1}	9.93×10^{-1}	9.92×10^{-1}	9.92×10^{-1}	9.92×10^{-1}	9.92×10^{-1}
2	5.56×10^{-2}	5.32×10^{-2}	5.18×10^{-2}	5.10×10^{-2}	5.07×10^{-2}	5.06×10^{-2}
3	2.17×10^{-2}	8.34×10^{-3}	3.23×10^{-3}	1.21×10^{-3}	4.36×10^{-4}	2.95×10^{-4}
4	2.16×10^{-2}	8.21×10^{-3}	3.15×10^{-3}	1.19×10^{-3}	4.34×10^{-4}	1.55×10^{-4}
5	2.15×10^{-2}	8.19×10^{-3}	3.14×10^{-3}	1.18×10^{-3}	4.33×10^{-4}	1.55×10^{-4}

Table 2: Convergence of the (normalized) reduced basis bound gap $\max_{\mu \in \Xi \subset \mathcal{D}} (J_N^+(\mu) - J_N^-(\mu))/|J_{\text{ref}}(\mu)|$ for the linear elasticity problem with the number of degrees of freedom of the underlying $\mathbb{P}^3$ finite element discretization ($\mathcal{N}$) and the reduced basis space dimension (N). The reference value for *normalization* (and not *assessment per se*), $|J_{\text{ref}}(\mu)|$, is computed using a $\mathcal{N} = 591{,}745$ finite element solution.

uniform meshes. Our reduced basis space is constructed from the finite element solution evaluated at N Chebyshev-Lobatto nodes of $\mathcal{D}$ mapped by a logarithmic transformation. The reduced basis formulation exercises the extensions developed in Sections 3.1, 3.5, and 3.6. The number of terms in the affine expansion of the right-hand side (11) is $S = 1$; hence we may readily find the solution for any $N \geq 1$.

Unlike the reaction-diffusion problem considered in Section 4.1, the exact solution of this planar elasticity problem is not smooth; in particular, in the presence of the 90° corners with the fully-clamped and traction-free interfaces, the solution can be shown to be in $(H^{3/2+\epsilon}(\Omega))^2$, $\epsilon > 0$, for $\ell \in (L^2(\Omega))^2$ [14]. Hence, we will not attempt to compute the exact output for this case; we instead report the convergence of the bound gap, $J_N^+(\mu) - J_N^-(\mu)$, with the finite element resolution $\mathcal{N}$ and the reduced basis dimension N. Note that this is in fact the mode of operation for many complicated practical problems and is precisely when the rigorous bounds for infinite-dimensional variational problem is important: the computation of the "exact" solution is unreasonably expensive and yet we wish to have guaranteed certainty in our computation.

Table 2 shows the convergence of the maximum (normalized) bound gap over $\Xi \subset \mathcal{D}$, where the surrogate subset Ξ consists of 201 points equidistributed over $\mathcal{D}$ in the logarithmic sense. The bound gap is expressed a function of the physical space resolution (as reflected in $\mathcal{N}$) and the parameter space resolution (as reflected in N). For $N = 1$, the parameter space resolution limits the bound quality independent of the physical space resolution; for $\mathcal{N} = 175$, the bound quality is largely limited by the finite element resolution. We again observe, for $\mathcal{N} = 148{,}417$, a rapid initial convergence of the bound gap with N. Due to the spatial irregularity mentioned above, the convergence of the bound with the uniform mesh refinement is rather slow.

5. Summary and Discussions

We propose a reduced basis certification strategy that provides rigorous upper and lower bounds of the energy associated with the *exact* infinite-dimensional weak solution of parametrized steady symmetric coercive equations. The upper bound construction is based on the usual variational argument over a subspace; the lower bound construction is based on a reduced basis approximation of the dual variable that satisfies *exactly* the dual feasibility conditions. We then consider various extensions of the basic technology. The formulation yields truly rigorous certificates of the reduced basis energy prediction (and the energy norm of the solution) without any assumptions as regard the accuracy of the underlying finite element discretization.

We identify several future research directions that address some of the limitations noted in the Introduction. We also reference relevant past work developed in different contexts. First is the extension to coercive but nonsymmetric equations and to other functional output quantities; we refer to Sauer-Budge and Peraire [17] for the formulation in the finite element context. Second is the extension to noncoercive equations; we refer to the work of Peraire and Patera [11] for a related formulation which provides *asymptotic* bounds in the finite element context. Third is the extension to nonlinear equations; for a limited class of nonlinearities, it may be possible to incorporate the technique developed in Machiels *et al.* [8] in the finite element context. Fourth is the extension to nonaffine parameter dependence; we may incorporate the empirical interpolation method [2] and the associated error bounds [3]. Fifth is the simplification of the finite element equilibration procedure; we may incorporate certain discontinuous Galerkin methods which automatically produce equilibrated fluxes [19]. Sixth is the application to large-scale engineering systems; we may develop an approach similar to the component-based reduced-basis method [4]. Although all these extensions should in principle be possible, none is simple and furthermore the complementary energy approach is clearly most advantageous in the symmetric coercive context.

We also identify an important related development which is more widely applicable: an adaptation strategy that controls both the physical space error due to the lack of the finite-element resolution and parameter space error due to the lack of reduced-basis resolution. We note two recent work that demonstrate the effectiveness of spatial adaptivity in the reduced basis context: the work of Steih and Urban [18] which uses an adaptive wavelet discretization; our work which uses a minimum-residual mixed method [20]. The latter formulation is built on duality but not on complementary energy. In this adaptive context, we can consider a larger class of equations, as the emphasis is on the development of an optimal approximation even if we cannot confirm accuracy with complete rigor.

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